

6.2 CAPE-OPEN Thermo interface

**Experiences and how-to advice on
CAPE-OPEN THRM interface**



Outline

- ▼ Review main Thermo objects
- ▼ Interface diagram THRM 1.0
- ▼ Some clarifications
- ▼ Limitations of THRM 1.0 and THRM 1.1 goals
- ▼ Interface diagram THRM 1.1
- ▼ Implementation of THRM 1.1
- ▼ Review process



Main objects

▼ Material Object

▼ Thermo System (1.0) / Property Package Manager (1.1)

▼ Property Package (PP)

▼ Equilibrium Server (1.0) / Calculator (1.1)

▼ Calculation Routine (1.0) / Physical Property Calculator (1.1)



Material Object

▼ Container for properties of a material

- ⦿ Components
- ⦿ Phases
- ⦿ Pressure, temperature compositions
- ⦿ Other properties...
- ⦿ Reference to a Property Package (PP)

▼ Used by client of Property Package

- ⦿ To specify input for calculations
- ⦿ To collect output from calculations



Property Package (PP)

▼ Software component

↳ both a Physical Property Calculator and an Equilibrium Calculator for materials containing a specific set of compounds occurring in a specific number of physical states.

▼ Will make use of certain models to perform these calculations.

▼ Configurable to make use of external Physical Property Calculators and/or Equilibrium Calculators.

▼ Alternatively, it can provide the functionality of any or both of these two components internally without making use of external components.



Property Package (PP)

▼ Self-contained collection of

- ⦿ Chemical compounds (pure substances)
 - Defined through basic constants eg. T_c
 - Optionally data/correlations on T-dependent properties, eg. Vapour pressure
- ⦿ Models/correlations/data for mixture properties
 - Model parameters/Binary interaction parameters
- ⦿ Phases (1.0 and 1.1) / Physical states (1.1)
- ⦿ Equilibrium calculation procedures

▼ Targeted to a particular application

- ▼ May be stand-alone or handled by a Property Package Manager
- ▼ Normally contains a small subset of all the compounds and models available through a Property Package Manager.



Calculation Routine / Physical Prop Calculator

▼ Software component:

⇒ given the temperature, pressure and composition of a phase of a material, is able to calculate an additional property or properties of the material.

▼ Is designed to work with certain kinds of material.

▼ Is not called directly by a PME, rather, it is called via a Property Package.

▼ Purpose: extend or to override the list of calculations that a Property Package can perform.

▼ Can only be used with a Property Package supporting the use of Physical Property Calculators.



Equilibrium Server

▼ Software component:

⇒ given a description of a material, and a specification of constraints on the calculations such as temperature and pressure, can calculate the composition of each phase present in the material.

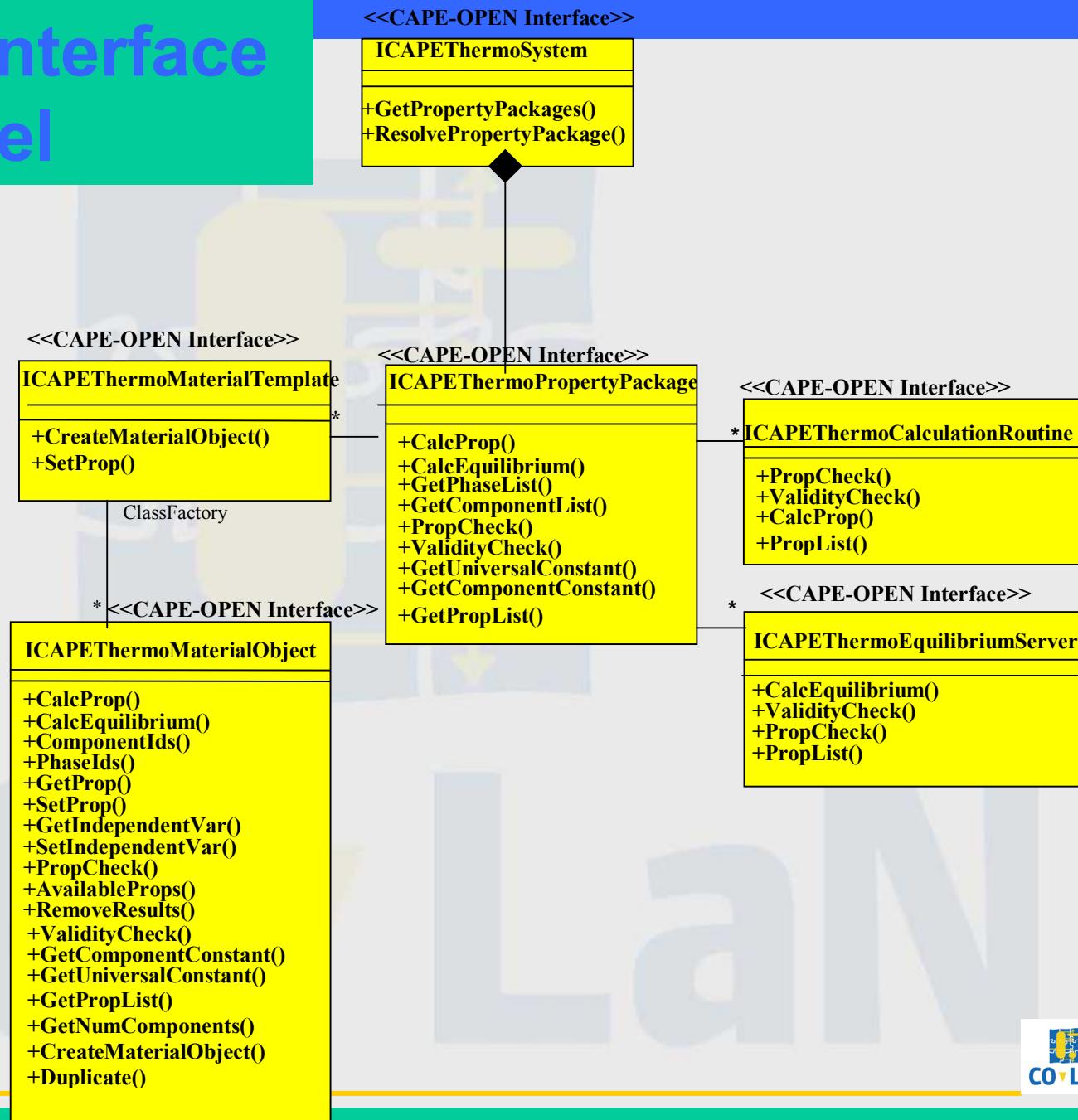
▼ May be implemented as part of PP or stand-alone.

▼ Always called through a PP.

▼ Provide specialist capabilities, e.g. Hydrate calculations.



THRM 1.0 interface model



Clarifications

▼ **On behavior expected by CAPE-OPEN software components:**

- ↪ Contract between a PMC and a PME

▼ **On interface specification**

- ↪ Some method descriptions are lacking details

▼ **On implementations issues**

- ↪ ProgIds names should not contain any blanks



Clarification on compound number and order

- ▼ A PP cannot assume anything at any time about the length or order of the compound list in an MO:
 - ➲ For example Aspen Plus will remove zero components from some calls that could eventually get directed to CAPE-OPEN Packages - but only for CalcProp calls not CalcEquilibrium.
 - ➲ This would happen on a per call basis.
- ▼ Number and order of compounds in MO to be checked by PP.



Clarification on derivatives

- ▼ For mole number derivatives of the fugacity coefficients: $f_{ij} = dfug_i/dn_j$
- ▼ Order should be $f_{11}, f_{21}, \dots, f_{n1}, f_{12}, f_{22}, \dots, f_{n2}, \dots f_{n1}, \dots, f_{nn}$
- ▼ So for 3 components the results are:
 $dF(1)/dN(1), dF(2)/dN(1), dF(3)/dN(1),$
 $dF(1)/dN(2), dF(2)/dN(2), dF(3)/dN(2),$
 $dF(1)/dN(3), dF(2)/dN(3), dF(3)/dN(3),$

Clarifications

- ▼ **Don't hesitate to ask for clarifications:**
→ **technologyofficer@colan.org**
- ▼ **Questions are circulated within the Thermo SIG.**
- ▼ **Easiest and quickest way to reach experts in THRM implementation: AspenTech, InfoChem, PPDS, ProSim, etc..**



Some limitations of THRM 1.0

- ▼ **Suitable mostly for vapor-liquid equilibrium**
 - ↪ Mapping phase names between a PP and a PME was an issue.

- ▼ **Reduced scope of equilibrium calculations:**
 - ↪ Fixed flash types.

- ▼ **Possible performance issues resolved**
 - ↪ i.e. lacked method to retrieve with one call temperature, pressure and composition.



Objectives of THRM 1.1

▼ Enhance functionality

↪ Phases

- Any number of phases
- Any types of phases

↪ Properties

- Constants (pure compounds)
- T/P-dependent properties (pure compounds)
- single-phase mixture properties
- 2-phase mixture properties

↪ Generalise flash specifications

▼ Enable/support efficient implementations



Objectives of THRM 1.1

▼ Make the specification a useful working document for developers

- ↪ Clarity
- ↪ Explain the purpose of each method
- ↪ Indicate how it is supposed to work
- ↪ Detailed description of arguments
- ↪ List of exceptions

▼ Logical classification of methods

- ↪ Enquiry (eg. GetSinglePhasePropList)
- ↪ Check (eg. CheckSinglePhasePropSpec)
- ↪ Calculate (eg. CalcSinglePhaseProp)



Thermo 1.1 Interface diagram

<<CAPE-OPEN Interface>>

ICAPEThermoPackageManager
+GetPropertyPackageList() +GetPropertyPackage()

<<CAPE-OPEN Interface>>

ICAPEThermoMaterial
+GetPresentPhases() +SetPresentPhases()
+GetSinglePhaseProp() +SetSinglePhaseProp()
+GetTwoPhaseProp() +SetTwoPhaseProp()
+GetOverallProp() +SetOverallProp()
+ClearAllProps() +GetTPFraction()
+CreateMaterial() +CopyFromMaterial()

<<CAPE-OPEN Interface>>

ICAPEThermoContext
+SetMaterial()

<<CAPE-OPEN Interface>>

ICAPEThermoPhases
+GetPhaseList() +GetPhaseInfo() +GetNumPhases()

<<CAPE-OPEN Interface>>

ICAPEThermoCompounds
+GetCompoundList() +GetCompoundConstant()
+GetConstPropList() +GetNumCompounds()
+GetPDependentProperty() +GetPDependentPropList()
+GetTDependentProperty() +GetTDependentPropList()

<<CAPE-OPEN Interface>>

ICAPEThermoPropertyRoutine
+CheckSinglePhasePropSpec() +GetSinglePhasePropList() +CalcSinglePhaseProp()
+CheckTwoPhasePropSpec() +GetTwoPhasePropList() +CalcTwoPhaseProp()
+CalcAndGetFugacityCoefficient()

<<CAPE-OPEN Interface>>

ICAPEThermoEquilibriumRoutine
+CheckEquilibriumSpec() +CalcEquilibrium()

<<CAPE-OPEN Interface>>

ICAPEThermoUniversalConstant
+GetUniversalConstant() +GetUniversalConstantList()



Implementing the 1.1 Standard as plug

▼ Prototype components by InfoChem

- ↪ Property Package
- ↪ Property Calculator

▼ Strategy

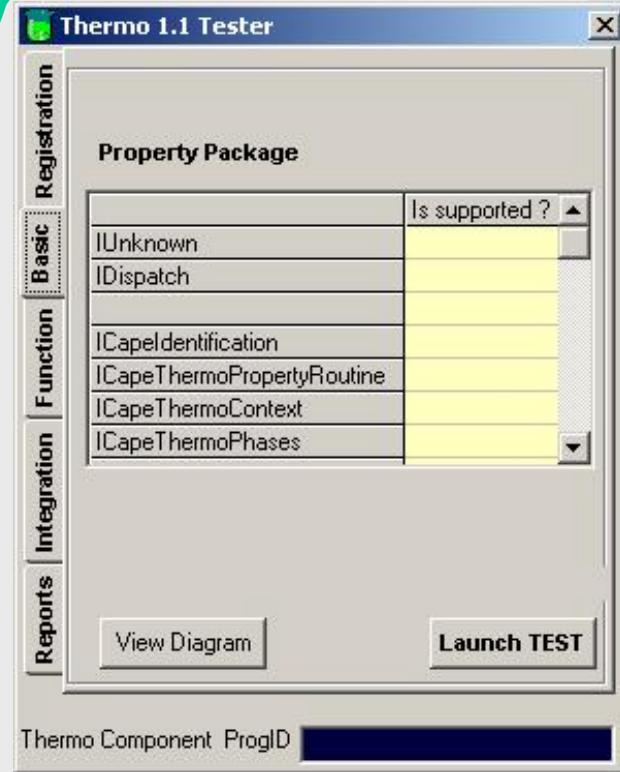
- ↪ VB code to implement the interfaces/methods
- ↪ Calculation engine as separate dll
- ↪ PP and PC do not contain any compound, phase or model-specific code

▼ Models etc.

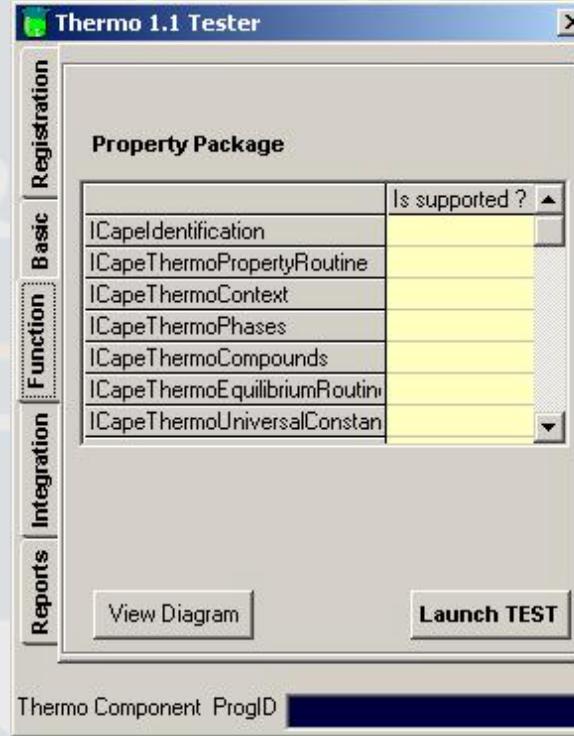
- ↪ RKS eos, viscosity from mixing rule
- ↪ Vapour, Liquid and AqueousLiquid phases
- ↪ 11 compounds
- ↪ PT and PH flash



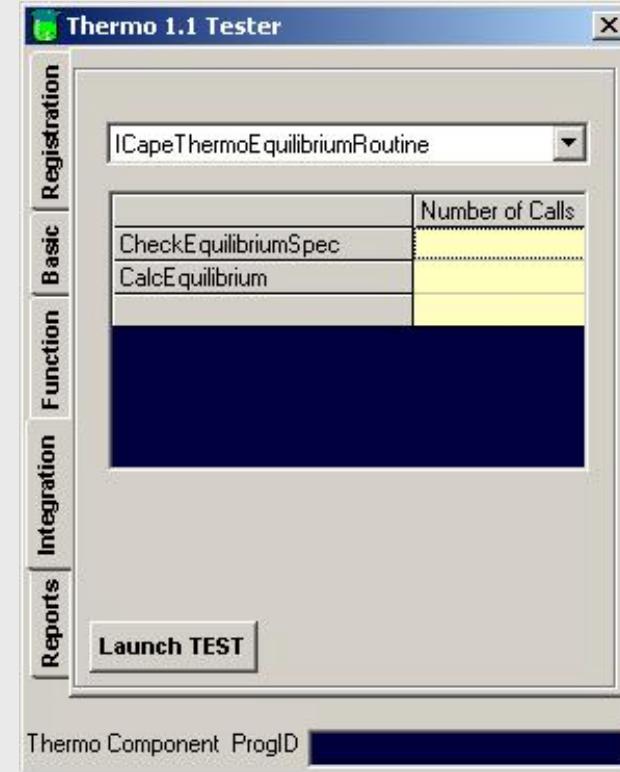
CO Tester: 1.1 socket by UPC



Basic Test



Function Test



Integration Test

Review process launched

- ▼ Draft specification published in April 2003
- ▼ Prototyped (May 03 till Feb 04) in:
 - ↪ CO-Tester
 - ↪ MultiFlash
- ▼ Implementation in:
 - ↪ SolidSim project (till March 05)
 - ↪ VMGThermo (released April 05)
 - ↪ Aspen Plus (2006)
- ▼ May 1, 2005: review launched within the Thermo SIG
- ▼ May 15, 2005: review by entire CO-LaN membership
- ▼ June 15, 2005: end of review → assessment by BOD





Join the THRM 1.1 review process!

CO²LaN

